

02/01/2005

10750247.trn

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1626GMS

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS	4	OCT 28	KOREAPAT now available on STN
NEWS	5	NOV 30	PHAR reloaded with additional data
NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS EXPRESS			OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS INTER			General Internet Information
NEWS LOGIN			Welcome Banner and News Items
NEWS PHONE			Direct Dial and Telecommunication Network Access to STN
NEWS WWW			CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 15:45:25 ON 02 JAN 2005

=>

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Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:45:36 ON 02 JAN 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 31 DEC 2004 HIGHEST RN 806622-48-0

DICTIONARY FILE UPDATES: 31 DEC 2004 HIGHEST RN 806622-48-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

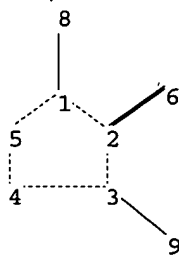
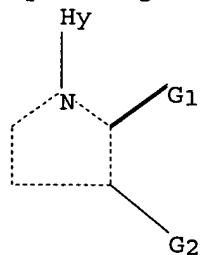
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10750247.str



chain nodes :

6 8 9

ring nodes :

1 2 3 4 5

chain bonds :

1-8 2-6 3-9

ring bonds :

1-2 1-5 2-3 3-4 4-5

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exact/norm bonds :

1-2 1-5 1-8 2-3 2-6 3-4 3-9 4-5

isolated ring systems :

containing 1 :

G1:O,S

G2:OH,NH2

Match level :

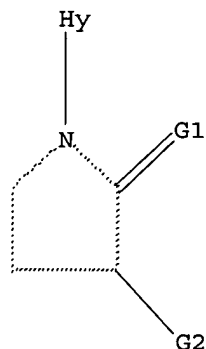
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 9:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O,S

G2 OH,NH2

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 15:45:52 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 5890 TO ITERATE

17.0% PROCESSED 1000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 113199 TO 122401  
PROJECTED ANSWERS: 19251 TO 23157

L2 50 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 15:46:09 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 117835 TO ITERATE

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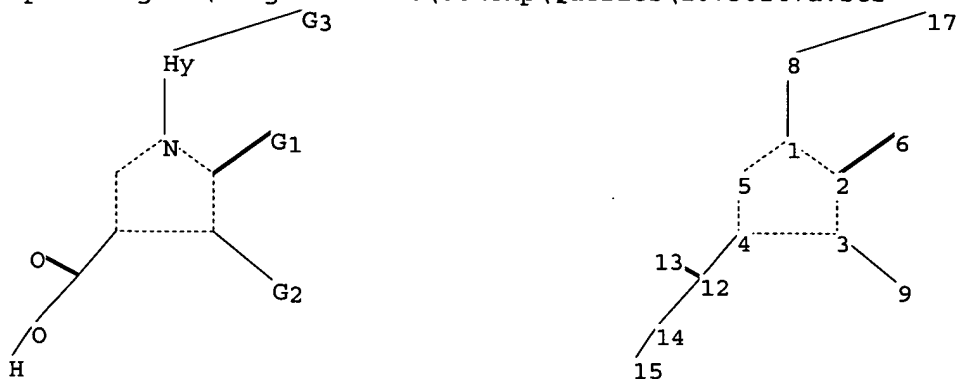
100.0% PROCESSED 117835 ITERATIONS  
SEARCH TIME: 00.00.06

21147 ANSWERS

L3 21147 SEA SSS FUL L1

=>

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chain nodes :

6 8 9 12 13 14 15 17

ring nodes :

1 2 3 4 5

chain bonds :

1-8 2-6 3-9 4-12 8-17 12-13 12-14 14-15

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-8 2-3 2-6 3-4 3-9 4-5 8-17

exact bonds :

4-12 14-15

normalized bonds :

12-13 12-14

isolated ring systems :

containing 1 :

G1:O,S

G2:OH,NH2

G3:OH,MeO,EtO,NH2,NO2,X,Ak,CN

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 9:CLASS 12:CLASS  
13:CLASS 14:CLASS 15:CLASS 17:CLASS

L4 STRUCTURE UPLOADED

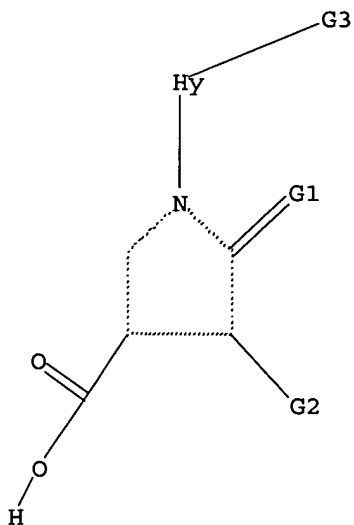
=> d 14

L4 HAS NO ANSWERS

L4 STR

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G1 O, S

G2 OH, NH2

G3 OH, MeO, EtO, NH2, NO2, X, Ak, CN

Structure attributes must be viewed using STN Express query preparation.

=> s l4

SAMPLE SEARCH INITIATED 15:52:00 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 56 TO ITERATE

100.0% PROCESSED 56 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 672 TO 1568  
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s l4 sss full

FULL SEARCH INITIATED 15:52:11 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1064 TO ITERATE

100.0% PROCESSED 1064 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

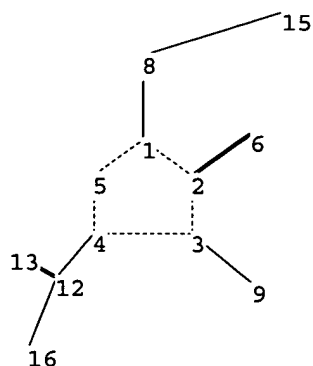
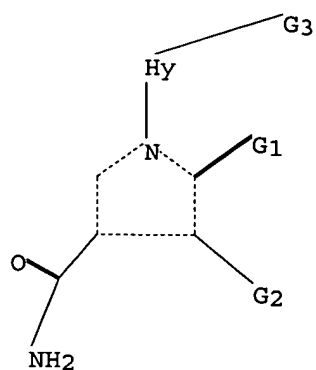
L6 0 SEA SSS FUL L4

=>

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chain nodes :

6 8 9 12 13 15 16

ring nodes :

1 2 3 4 5

chain bonds :

1-8 2-6 3-9 4-12 8-15 12-13 12-16

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-8 2-3 2-6 3-4 3-9 4-5 8-15 12-13 12-16

exact bonds :

4-12

isolated ring systems :

containing 1 :

G1:O,S

G2:OH,NH2

G3:OH,MeO,EtO,NH2,NO2,X,Ak,CN

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 9:CLASS 12:CLASS

13:CLASS 15:CLASS 16:CLASS

L7 STRUCTURE UPLOADED

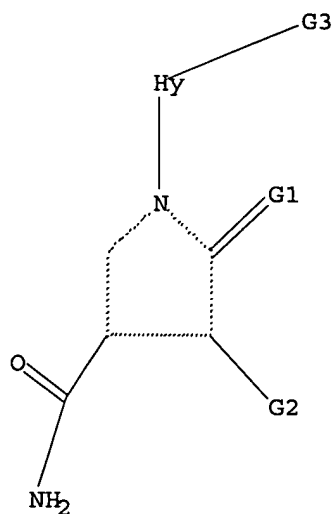
=> d 17

L7 HAS NO ANSWERS

L7 STR

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G1 O,S

G2 OH,NH<sub>2</sub>

G3 OH,MeO,EtO,NH<sub>2</sub>,NO<sub>2</sub>,X,Ak,CN

Structure attributes must be viewed using STN Express query preparation.

=> s 17

SAMPLE SEARCH INITIATED 15:54:10 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 60 TO ITERATE

100.0% PROCESSED 60 ITERATIONS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 736 TO 1664  
PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 17 sss full

FULL SEARCH INITIATED 15:54:16 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1244 TO ITERATE

100.0% PROCESSED 1244 ITERATIONS  
SEARCH TIME: 00.00.01

L9 0 SEA SSS FUL L7

=>

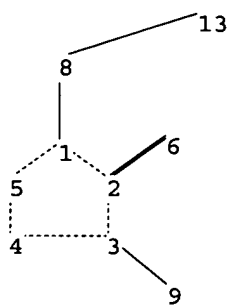
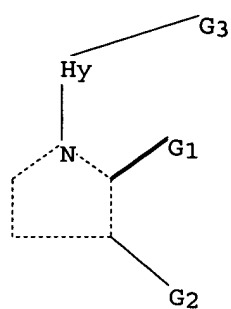
Uploading C:\Program Files\Stnexp\Queries\10750247c.str

0 ANSWERS

0 ANSWERS

02/01/2005

10750247.trn



chain nodes :

6 8 9 13

ring nodes :

1 2 3 4 5

chain bonds :

1-8 2-6 3-9 8-13

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-8 2-3 2-6 3-4 3-9 4-5 8-13

isolated ring systems :

containing 1 :

G1:O,S

G2:OH,NH2

G3:OH,MeO,EtO,NH2,NO2,X,Ak,CN

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 9:CLASS 13:CLASS

L10 STRUCTURE UPLOADED

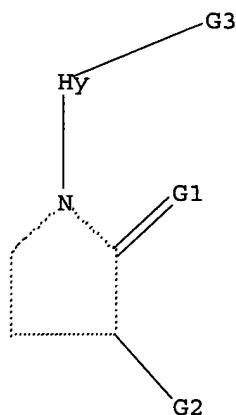
=> d l10

L10 HAS NO ANSWERS

L10 STR

02/01/2005

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G1 O,S

G2 OH,NH2

G3 OH,MeO,EtO,NH2,NO2,X,Ak,CN

Structure attributes must be viewed using STN Express query preparation.

=> s l10

SAMPLE SEARCH INITIATED 15:55:41 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 5890 TO ITERATE

17.0% PROCESSED 1000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 113199 TO 122401  
PROJECTED ANSWERS: 13098 TO 16352

L11 50 SEA SSS SAM L10

=> s l10 sss full

FULL SEARCH INITIATED 15:56:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 117835 TO ITERATE

100.0% PROCESSED 117835 ITERATIONS  
SEARCH TIME: 00.00.06

13892 ANSWERS

L12 13892 SEA SSS FUL L10

=> d his

(FILE 'HOME' ENTERED AT 15:45:25 ON 02 JAN 2005)

FILE 'REGISTRY' ENTERED AT 15:45:36 ON 02 JAN 2005

L1 STRUCTURE UPLOADED  
L2 50 S L1  
L3 21147 S L1 SSS FULL  
L4 STRUCTURE UPLOADED  
L5 0 S L4

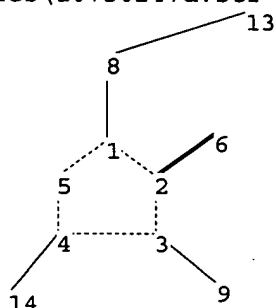
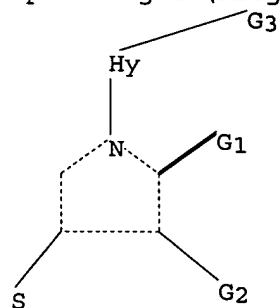
02/01/2005

10750247.trn

L6 0 S L4 SSS FULL  
L7 STRUCTURE UPLOADED  
L8 0 S L7  
L9 0 S L7 SSS FULL  
L10 STRUCTURE UPLOADED  
L11 50 S L10  
L12 13892 S L10 SSS FULL

=>

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chain nodes :  
6 8 9 13 14  
ring nodes :  
1 2 3 4 5  
chain bonds :  
1-8 2-6 3-9 4-14 8-13  
ring bonds :  
1-2 1-5 2-3 3-4 4-5  
exact/norm bonds :  
1-2 1-5 1-8 2-3 2-6 3-4 3-9 4-5 4-14 8-13  
isolated ring systems :  
containing 1 :

G1:O,S

G2:OH,NH2

G3:OH,MeO,EtO,NH2,NO2,X,Ak,CN

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 9:CLASS 13:CLASS  
14:CLASS

L13 STRUCTURE UPLOADED

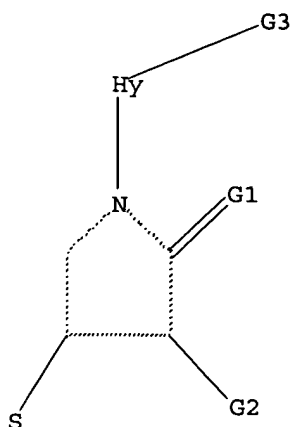
=> d l13

L13 HAS NO ANSWERS

L13 STR

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G1 O,S

G2 OH,NH2

G3 OH,MeO,EtO,NH2,NO2,X,Ak,CN

Structure attributes must be viewed using STN Express query preparation.

=> s l13

SAMPLE SEARCH INITIATED 15:58:21 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 315 TO ITERATE

100.0% PROCESSED 315 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 5236 TO 7364

PROJECTED ANSWERS: 0 TO 0

L14 0 SEA SSS SAM L13

=> s l13 sss full

FULL SEARCH INITIATED 15:58:28 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 6419 TO ITERATE

100.0% PROCESSED 6419 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

L15 2 SEA SSS FUL L13

=> d his

(FILE 'HOME' ENTERED AT 15:45:25 ON 02 JAN 2005)

FILE 'REGISTRY' ENTERED AT 15:45:36 ON 02 JAN 2005

L1 STRUCTURE UPLOADED

L2 50 S L1

L3 21147 S L1 SSS FULL

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 0 S L4 SSS FULL

02/01/2005

10750247.trn

L7 STRUCTURE UPLOADED  
L8 0 S L7  
L9 0 S L7 SSS FULL  
L10 STRUCTURE UPLOADED  
L11 50 S L10  
L12 13892 S L10 SSS FULL  
L13 STRUCTURE UPLOADED  
L14 0 S L13  
L15 2 S L13 SSS FULL

FIL CAPLUS

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
813.96	814.17

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 15:58:58 ON 02 JAN 2005  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 2 Jan 2005 VOL 142 ISS 2  
FILE LAST UPDATED: 31 Dec 2004 (20041231/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> S 115

L16 1 L15

=> d 116 ibib abs hitstr tot

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:777806 CAPLUS

DOCUMENT NUMBER: 139:292253

TITLE: Preparation of novel dithiolopyrrolones with therapeutic activity against proliferative diseases

INVENTOR(S): Chen, Genhui; Li, Bin; Li, Jianxiong; Webster, John

PATENT ASSIGNEE(S): Weirchem Biotech Inc., Can.

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003080624	A2	20031002	WO 2003-CA380	20030318

WO 2003080624

A3

20040325

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1490374

A2

20041229

EP 2003-744744

20030318

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.:

US 2002-367265P

P 20020326

US 2002-418698P

P 20021017

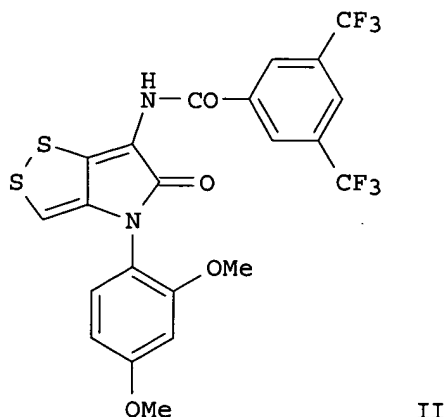
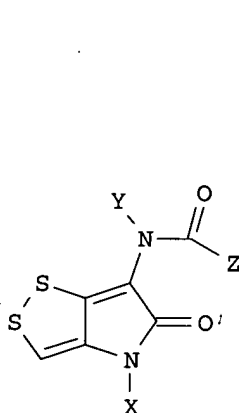
WO 2003-CA380

W 20030318

OTHER SOURCE(S):

MARPAT 139:292253

GI



AB The present invention provides novel dithiolopyrrolone compds. (I) [X and Y can be the same or different, are hydrogen, substituted or unsubstituted alkyl, cycloalkyl, aryl, aralkyl or heterocyclic group except the compds. with: Z = Ph, Y = H, X = H, Me or benzyl, and Z = 4-pyridine, X = Me, Y = H; or When X = aryl, heterocyclic, Y and Z, can be the same or different, are hydrogen, unsubstituted or substituted or alkyl of two or less hydroxy groups and no carboxylic acid group, cycloalkyl, aryl, aralkyl or heterocyclic group, except the compds. with: Z = Me, Y = H, X = Ph, 4-methoxyphenyl, 4-methylphenyl] and their salts, which are useful as treatments for cancer and other proliferative diseases. The present invention also provides therapeutic compns. comprising particularly useful types of dithiolopyrrolones, the salts thereof, and methods of using the compds. within such types, particularly in treating proliferative diseases such as cancer. For example, 1,2-dithiolo[4,3-b]pyrrol-5(4H)-one derivative (II) in vitro showed IC<sub>50</sub> of ≤0.01, 0.13, 0.016, 0.14, 0.014, 0.03, 0.04, 0.013, and 0.013 μM against leukemia CCRF-CEM, non-small cell lung cancer, colon cancer HCT-116, CNS cancer 0.14, melanoma LOXIMVI, ovarian cancer OVCAR-3, renal cancer RXF 393, prostate cancer DU-145, and breast cancer T-47D, resp.

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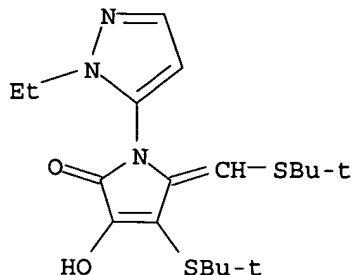
IT 608132-09-8P 608132-18-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of novel dithiolopyrrolones with therapeutic activity against proliferative diseases such as cancer)

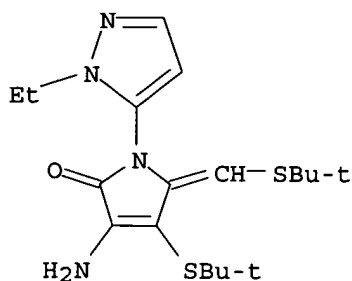
RN 608132-09-8 CAPLUS

CN 2H-Pyrrol-2-one, 4-[(1,1-dimethylethyl)thio]-5-[[[(1,1-dimethylethyl)thio]methylene]-1-(1-ethyl-1H-pyrazol-5-yl)-1,5-dihydro-3-hydroxy- (9CI) (CA INDEX NAME)



RN 608132-18-9 CAPLUS

CN 2H-Pyrrol-2-one, 3-amino-4-[(1,1-dimethylethyl)thio]-5-[[[(1,1-dimethylethyl)thio]methylene]-1-(1-ethyl-1H-pyrazol-5-yl)-1,5-dihydro- (9CI) (CA INDEX NAME)



=> s l12

L17 30 L12

=> s l15

L18 1 L15

=> s l17 and py<=2001

21605436 PY<=2001

L19 17 L17 AND PY<=2001

=> s l19 and thu

139 THU

2205406 THUS

2205530 THU

(THU OR THUS)

L20 3 L19 AND THU

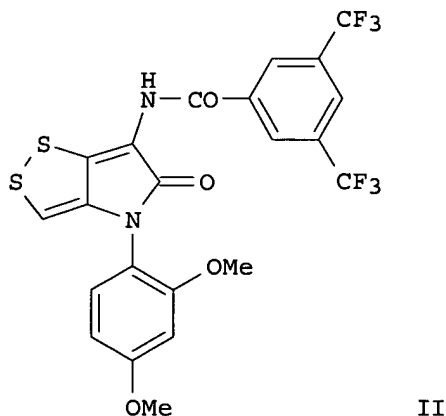
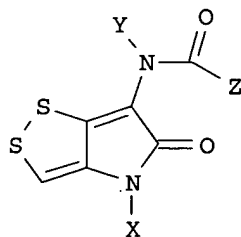
02/01/2005

10750247.trn

=&gt; d 118 ibib abs hitstr tot

L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2003:777806 CAPLUS  
DOCUMENT NUMBER: 139:292253  
TITLE: Preparation of novel dithiolopyrrolones with  
therapeutic activity against proliferative diseases  
INVENTOR(S): Chen, Genhui; Li, Bin; Li, Jianxiong; Webster, John  
PATENT ASSIGNEE(S): Wellchem Biotech Inc., Can.  
SOURCE: PCT Int. Appl., 33 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003080624	A2	20031002	WO 2003-CA380	20030318
WO 2003080624	A3	20040325		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1490374	A2	20041229	EP 2003-744744	20030318
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
PRIORITY APPLN. INFO.:			US 2002-367265P	P 20020326
			US 2002-418698P	P 20021017
			WO 2003-CA380	W 20030318
OTHER SOURCE(S):	MARPAT 139:292253			
GI				



AB The present invention provides novel dithiolopyrrolone compds. (I) [X and Y can be the same or different, are hydrogen, substituted or unsubstituted alkyl, cycloalkyl, aryl, aralkyl or heterocyclic group except the compds. with: Z = Ph, Y = H, X = H, Me or benzyl, and Z = 4-pyridine, X = Me, Y = H; or When X = aryl, heterocyclic, Y and Z, can be the same or different, are hydrogen, unsubstituted or substituted or alkyl of two or less hydroxy groups and no carboxylic acid group, cycloalkyl, aryl, aralkyl or heterocyclic group, except the compds. with: Z = Me, Y = H, X = Ph, 4-methoxyphenyl, 4-methylphenyl] and their salts, which are useful as treatments for cancer and other proliferative diseases. The present invention also provides therapeutic compns. comprising particularly useful types of dithiolopyrrolones, the salts thereof, and methods of using the compds. within such types, particularly in treating proliferative diseases such as cancer. For example, 1,2-dithiolo[4,3-b]pyrrol-5(4H)-one derivative (II) in vitro showed IC<sub>50</sub> of  $\leq 0.01$ , 0.13, 0.016, 0.14, 0.014, 0.03, 0.04, 0.013, and 0.013  $\mu\text{M}$  against leukemia CCRF-CEM, non-small cell lung cancer, colon cancer HCT-116, CNS cancer 0.14, melanoma LOXIMVI, ovarian cancer OVCAR-3, renal cancer RXF 393, prostate cancer DU-145, and breast cancer T-47D, resp.

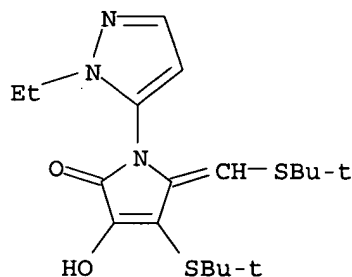
IT 608132-09-8P 608132-18-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of novel dithiolopyrrolones with therapeutic activity against proliferative diseases such as cancer)

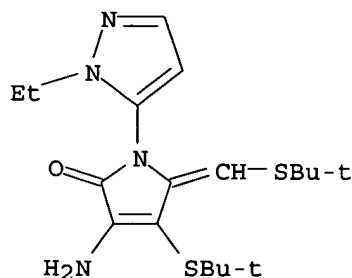
RN 608132-09-8 CAPLUS

CN 2H-Pyrrol-2-one, 4-[(1,1-dimethylethyl)thio]-5-[[[(1,1-dimethylethyl)thio]methylene]-1-(1-ethyl-1H-pyrazol-5-yl)-1,5-dihydro-3-hydroxy- (9CI) (CA INDEX NAME)



RN 608132-18-9 CAPLUS

CN 2H-Pyrrol-2-one, 3-amino-4-[(1,1-dimethylethyl)thio]-5-[[[(1,1-dimethylethyl)thio]methylene]-1-(1-ethyl-1H-pyrazol-5-yl)-1,5-dihydro- (9CI) (CA INDEX NAME)



02/01/2005

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L19 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:247333 CAPLUS

DOCUMENT NUMBER: 134:266475

TITLE: Preparation of quinuclidine compounds and drugs containing the same as the active ingredient of squalene synthase inhibitors

INVENTOR(S): Okada, Toshimi; Kurusu, Nobuyuki; Tanaka, Keigo; Miyazaki, Kazuki; Shinmyo, Daisuke; Sugumi, Hiroyuki; Ikuta, Hironori; Hiyoshi, Hironobu; Saeki, Takao; Yanagimachi, Mamoru; Ito, Masashi

PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan; et al.

SOURCE: PCT Int. Appl., 267 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

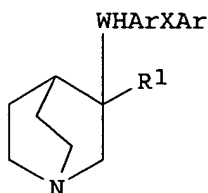
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

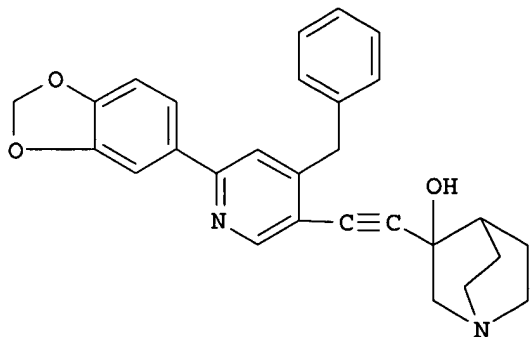
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001023383	A1	20010405	WO 2000-JP6665	20000927 <--
W: AU, BR, CA, CN, HU, IL, JP, KR, MX, NO, NZ, RU, US, ZA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2385995	AA	20010405	CA 2000-2385995	20000927 <--
AU 2000074464	A5	20010430	AU 2000-74464	20000927 <--
EP 1217001	A1	20020626	EP 2000-962889	20000927
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
BR 2000014331	A	20030610	BR 2000-14331	20000927
NZ 517788	A	20031128	NZ 2000-517788	20000927
ZA 2002002034	A	20030312	ZA 2002-2034	20020312
US 6599917	B1	20030729	US 2002-88554	20020319
NO 2002001528	A	20020528	NO 2002-1528	20020326
PRIORITY APPLN. INFO.:			JP 1999-273905	A 19990928
			JP 2000-179352	A 20000615
			WO 2000-JP6665	W 20000927

OTHER SOURCE(S): MARPAT 134:266475

GI



I



II

AB Title compds. [I; wherein R1 is hydrogen or hydroxyl; HAr is an optionally substituted aromatic heterocycle; Ar is an optionally substituted aromatic ring;

W is a CH<sub>2</sub>CH<sub>2</sub> group which may be substituted, a CH:CH group which may be substituted, CC, NHCO, or the like; X is a single bond, optionally substituted C1-6 alkylene, Q ;wherein Q is oxygen, sulfur, CO, N(R<sub>2</sub>) ; wherein R<sub>2</sub> is C1-6 alkyl or C1-6 alkoxy, NHCO, or the like], salts thereof, or hydrates of both, are prepared and are useful as excellent squalene synthase inhibitors. Thus, the title compound II was prepared and tested.

IT 332132-83-9P

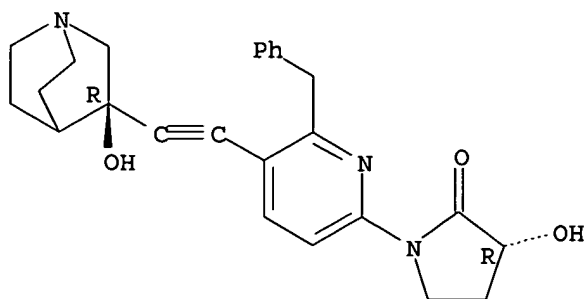
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinuclidine compds. and drugs containing the same as active ingredient of squalene synthase inhibitors)

RN 332132-83-9 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[5-[[ (3R)-3-hydroxy-1-azabicyclo[2.2.2]oct-3-yl]ethynyl]-6-(phenylmethyl)-2-pyridinyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 332135-05-4P 332135-10-1P

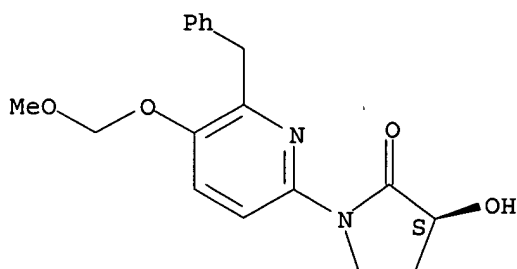
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of quinuclidine compds. and drugs containing the same as active ingredient of squalene synthase inhibitors)

RN 332135-05-4 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[5-(methoxymethoxy)-6-(phenylmethyl)-2-pyridinyl]-, (3S)- (9CI) (CA INDEX NAME)

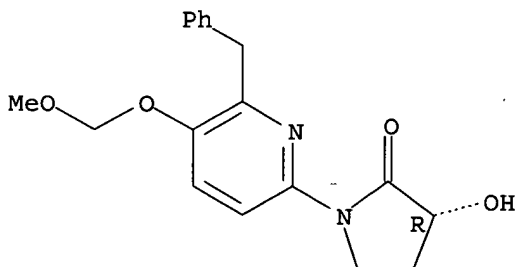
Absolute stereochemistry.



RN 332135-10-1 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[5-(methoxymethoxy)-6-(phenylmethyl)-2-pyridinyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 332132-82-8P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinuclidine compds. and drugs containing the same as active ingredient of squalene synthase inhibitors)

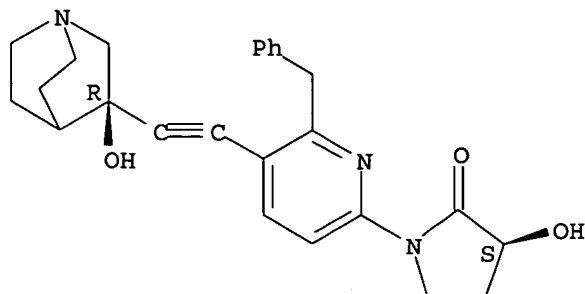
02/01/2005

10750247.trn

RN 332132-82-8 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[5-[[[(3R)-3-hydroxy-1-azabicyclo[2.2.2]oct-3-yl]ethynyl]-6-(phenylmethyl)-2-pyridinyl]-, (3S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:260235 CAPLUS

DOCUMENT NUMBER: 132:293663

TITLE: Preparation of cyclopropylcarbonylaminopyrrolidinones, -thiazolidinones, or -oxazolidinones as herbicides.

INVENTOR(S): Parry, David Rees; Matthews, Ian Richard; Mitchell, Glynn; Williams, Alfred Glyn; Barnes, Nigel John; Cox, John Michael; Gillen, Kevin James; Ensminger, Michael Paul; Khodayari, Khosro; Nakayama, Hiroto

PATENT ASSIGNEE(S): Zeneca Limited, UK

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

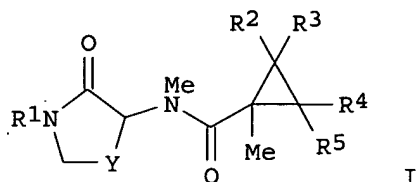
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000021928	A1	20000420	WO 1999-GB3143	19990921 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9961033	A1	20000501	AU 1999-61033	19990921 <--
BR 9914342	A	20010626	BR 1999-14342	19990921 <--
JP 2002527420	T2	20020827	JP 2000-575837	19990921
PRIORITY APPLN. INFO.:			GB 1998-22116	A 19981009
			WO 1999-GB3143	W 19990921

OTHER SOURCE(S): MARPAT 132:293663

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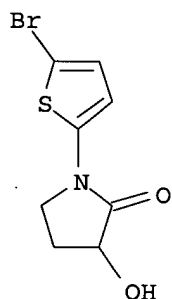


AB Title compds. [I; Y = O, S, CH<sub>2</sub>; R<sub>1</sub> = (substituted) aryl, heteroarom.; R<sub>2</sub>, R<sub>3</sub> = H, halogen; R<sub>4</sub>, R<sub>5</sub> = halo], were prepared Thus, 3-methylamino-1-(3-difluoromethoxy-4-methylphenyl)pyrrolidin-2-one (preparation given) in CH<sub>2</sub>Cl<sub>2</sub> was treated with 2,2-dichloro-1-methylcyclopropylcarbonyl chloride and then with Et<sub>3</sub>N to give diastereomeric 3-[N-(2,2-dichloro-1-methylcyclopropylcarbonyl)methylamino]-1-(3-difluoromethoxy-4-methylphenyl)pyrrolidin-2-one. Several I at 250 ppm preemergent gave 90-100% damage to *Amaranthus retroflexus*, *Echinochloa crus-galli*, etc.

IT **264194-57-2P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of cyclopropylcarbonylaminopyrrolidinones, -thiazolidinones, or -oxazolidinones as herbicides)

RN 264194-57-2 CAPLUS

CN 2-Pyrrolidinone, 1-(5-bromo-2-thienyl)-3-hydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:161902 CAPLUS

DOCUMENT NUMBER: 128:243903

TITLE: Synthesis and antibacterial activity of 1-substituted 5-aryl-4-aryl-3-hydroxy-3-pyrrolidin-2-ones

AUTHOR(S): Gein, V. L.; Pitirimova, S. G.; Voronina, E. V.; Porseva, N. Yu.; Pantsurkin, V. I.

CORPORATE SOURCE: Perm. Far. Akad., Perm, Russia

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1997), 31(11), 35-36

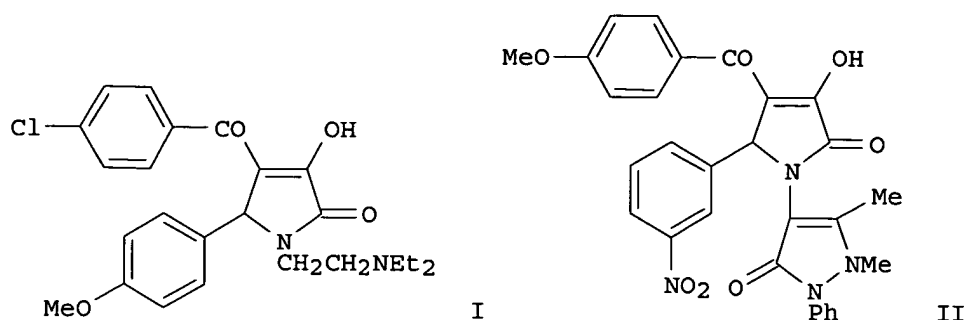
CODEN: KHFZAN; ISSN: 0023-1134

PUBLISHER: Izdatel'stvo Folium

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI



AB Title compds. such as I and II were prepared by cyclocondensation of Me 4-aryl-2,4-dioxobutanoates with benzaldehydes and either Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> or 4-aminoantipyrine. Several of the products or their hydrochlorides were tested against *Staphylococcus aureus* and *Escherichia coli*. The antipyrine moiety conferred no increase in antibacterial activity on these compds.

IT 204756-95-6P 204756-96-7P 204756-97-8P

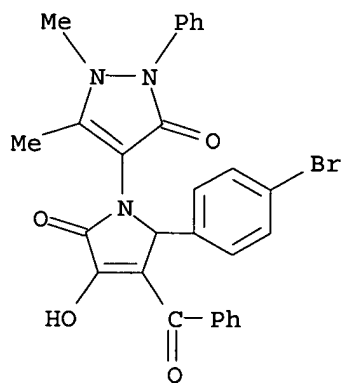
204757-02-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antibacterial activity of)

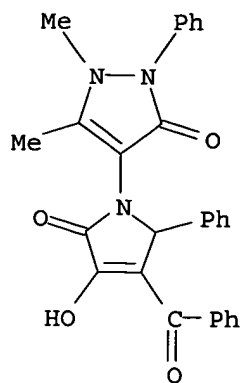
RN 204756-95-6 CAPLUS

CN 3H-Pyrazol-3-one, 4-[3-benzoyl-2-(4-bromophenyl)-2,5-dihydro-4-hydroxy-5-oxo-1H-pyrrol-1-yl]-1,2-dihydro-1,5-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)



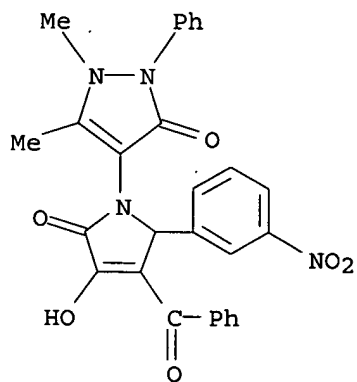
RN 204756-96-7 CAPLUS

CN 3H-Pyrazol-3-one, 4-(3-benzoyl-2,5-dihydro-4-hydroxy-5-oxo-2-phenyl-1H-pyrrol-1-yl)-1,2-dihydro-1,5-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)



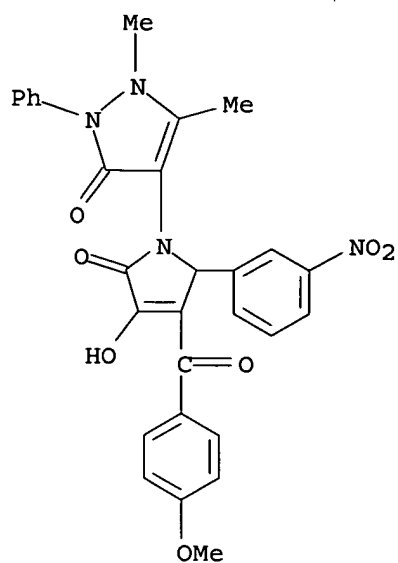
RN 204756-97-8 CAPLUS

CN 3H-Pyrazol-3-one, 4-[3-benzoyl-2,5-dihydro-4-hydroxy-2-(3-nitrophenyl)-5-oxo-1H-pyrrol-1-yl]-1,2-dihydro-1,5-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)



RN 204757-02-8 CAPLUS

CN 3H-Pyrazol-3-one, 4-[2,5-dihydro-3-hydroxy-4-(4-methoxybenzoyl)-5-(3-nitrophenyl)-2-oxo-1H-pyrrol-1-yl]-1,2-dihydro-1,5-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)



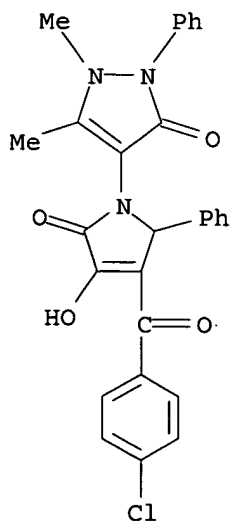
IT 204756-98-9P 204756-99-0P 204757-00-6P

204757-01-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

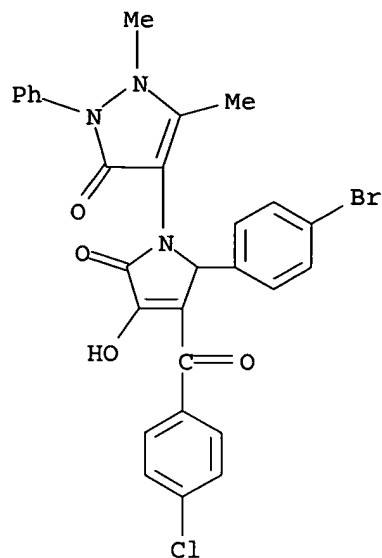
RN 204756-98-9 CAPLUS

CN 3H-Pyrazol-3-one, 4-[3-(4-chlorobenzoyl)-2,5-dihydro-4-hydroxy-5-oxo-2-phenyl-1H-pyrrol-1-yl]-1,2-dihydro-1,5-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)



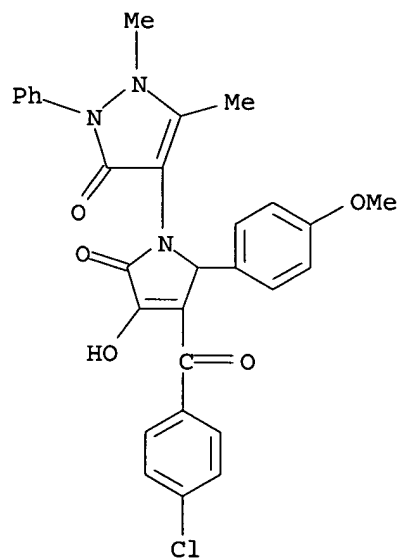
RN 204756-99-0 CAPLUS

CN 3H-Pyrazol-3-one, 4-[2-(4-bromophenyl)-3-(4-chlorobenzoyl)-2,5-dihydro-4-hydroxy-5-oxo-1H-pyrrol-1-yl]-1,2-dihydro-1,5-dimethyl-2-phenyl- (9CI)  
(CA INDEX NAME)



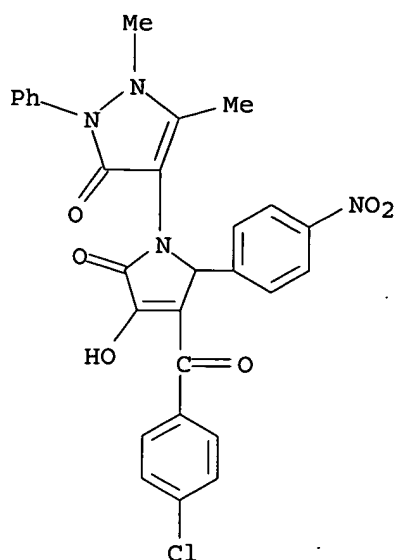
RN 204757-00-6 CAPLUS

CN 3H-Pyrazol-3-one, 4-[3-(4-chlorobenzoyl)-2,5-dihydro-4-hydroxy-2-(4-methoxyphenyl)-5-oxo-1H-pyrrol-1-yl]-1,2-dihydro-1,5-dimethyl-2-phenyl-  
(9CI) (CA INDEX NAME)



RN 204757-01-7 CAPLUS

CN 3H-Pyrazol-3-one, 4-[3-(4-chlorobenzoyl)-2,5-dihydro-4-hydroxy-2-(4-nitrophenyl)-5-oxo-1H-pyrrol-1-yl]-1,2-dihydro-1,5-dimethyl-2-phenyl-  
(9CI) (CA INDEX NAME)



L19 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:200115 CAPLUS

DOCUMENT NUMBER: 124:261022

TITLE: Preparation of substituted pyrrolidones, thiazolidones, or oxazolidones as herbicides

INVENTOR(S): Cox, John Michael; Clough, John Martin; Barnes, Nigel John; Pearson, David Philip John; Matthews, Ian Richard; Vohra, Shaheen Khatoon; Smith, Stephen Christopher; Mitchell, Glynn; Barber, Richard Anthony; Et, Al.

PATENT ASSIGNEE(S): Zeneca Ltd., UK

SOURCE: PCT Int. Appl., 221 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9533719	A1	19951214	WO 1995-GB1224	19950526 <--
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, FI, GE, HU, IS, JP, KP, KR, KZ, LK, LT, LV, MD, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2190979	AA	19951214	CA 1995-2190979	19950526 <--
AU 9525720	A1	19960104	AU 1995-25720	19950526 <--
AU 696084	B2	19980903		
EP 763020	A1	19970319	EP 1995-920158	19950526 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
HU 75808	A2	19970528	HU 1996-3248	19950526 <--
CN 1153512	A	19970702	CN 1995-194250	19950526 <--
BR 9507838	A	19970916	BR 1995-7838	19950526 <--
JP 10500985	T2	19980127	JP 1995-500502	19950526 <--

02/01/2005

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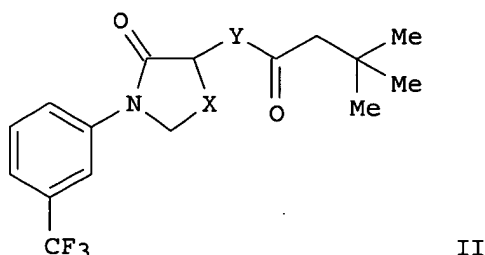
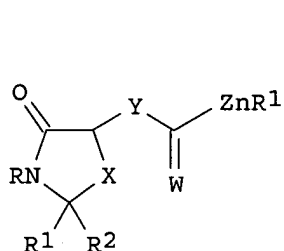
ZA 9504443  
CN 1341594  
PRIORITY APPLN. INFO.:

A 19960205  
A 20020327

ZA 1995-4443  
CN 2001-125418  
GB 1994-10998  
GB 1994-11004  
GB 1995-1158  
WO 1995-GB1224

19950531 <--  
20010815  
A 19940602  
A 19940602  
A 19950120  
W 19950526

OTHER SOURCE(S): MARPAT 124:261022  
GI



AB Title compds. [I; R = (un)substituted (hetero)aryl; R1 = H, hydrocarbyl, heterocyclyl, etc.; R2,R3 = H, alkyl; W = O or S; X = O, S, CR4R5; R4,R5 = H, alkyl; Y = O, S, NR6, CR4R5, etc.; R6 = H, OH, CHO, (di)(hydrocarbyl)amino, hydrocarbyl, etc.; Z = O, S, NR4, etc.; n = 0 or 1] were prepared. Thus, 3-(F3C)C6H4NH2 was cyclocondensed with HSCH2CO2H and HCHO and the product converted in 2 steps to 5-hydroxy-3-(3-trifluoromethylphenyl)-4-thiazolidinone which was O-acylated with Me3CCH2COC1 to give title compound II (X = S, Y = O). II (X = CH2, Y = NH) gave 90-100% control of 7 weeds, e.g., Amaranthus retroflexus, with 6-15% damage to soybean and corn and no damage to rice at 500g/ha preemergent.

IT 174889-59-9P 174889-68-0P 174889-87-3P

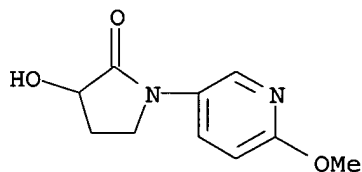
174889-88-4P 174889-89-5P 174889-90-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted pyrrolidones, thiazolidones, or oxazolidones as herbicides)

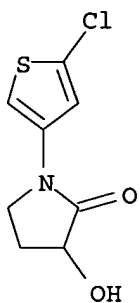
RN 174889-59-9 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-(6-methoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)



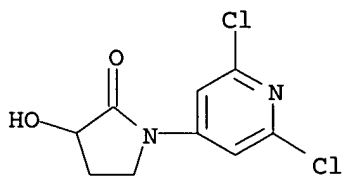
RN 174889-68-0 CAPLUS

CN 2-Pyrrolidinone, 1-(5-chloro-3-thienyl)-3-hydroxy- (9CI) (CA INDEX NAME)



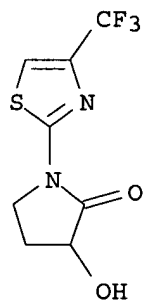
RN 174889-87-3 CAPLUS

CN 2-Pyrrolidinone, 1-(2,6-dichloro-4-pyridinyl)-3-hydroxy- (9CI) (CA INDEX NAME)



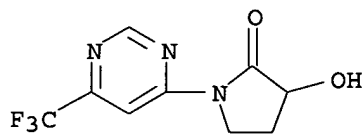
RN 174889-88-4 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[4-(trifluoromethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



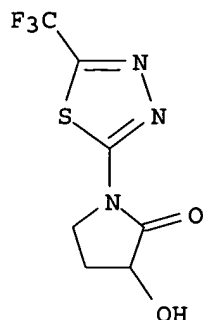
RN 174889-89-5 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[6-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 174889-90-8 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]- (9CI) (CA INDEX NAME)



L19 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:307859 CAPLUS

DOCUMENT NUMBER: 122:122445

TITLE: Side-chain hydroxylation in the metabolism of 8-aminoquinoline antiparasitic agents

AUTHOR(S): Idowu, O. R.; Peggs, J. O.; Brewer, T. G.

CORPORATE SOURCE: Department Pharmacology, Walter Reed Army Institute Research, Washington, DC, 20307-5100, USA

SOURCE: Drug Metabolism and Disposition (1995), 23(1), 18-27

CODEN: DMDSAI; ISSN: 0090-9556

PUBLISHER: Williams & Wilkins

DOCUMENT TYPE: Journal

LANGUAGE: English

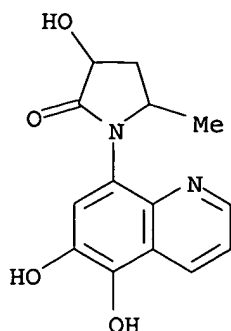
AB Primaquine, 8-(4-amino-1-methylbutylamino)-6-methoxyquinoline, is an antimalarial 8-aminoquinoline derivative. Although it has been in use since 1952, its metabolism has not been clearly defined. This is due to the instability of the expected aminophenol metabolites and their amphoteric nature, which makes their isolation difficult. Recent studies on the metabolism of WR 238605, a new primaquine analog, has shown that these problems may be solved by extracting the metabolites in the presence of Et chloroformate. Subsequent identification of the ethoxycarbonyl derivs. of the metabolites has made it possible to define the in vitro metabolism of primaquine. The primary metabolic pathways of primaquine involved hydroxylation of the Ph ring of the quinoline nucleus and C-hydroxylation of the 3'-position of the 8-aminoalkylamino side chain. Ring-hydroxylation of primaquine gives rise to 5-hydroxyprimaquine, which on demethylation produces 5-hydroxy-6-demethylprimaquine. Side-chain hydroxylation of primaquine gives rise to 3'-hydroxyprimaquine, which also undergoes O-demethylation to 3'-hydroxy-6-demethylprimaquine. 6-Demethylprimaquine, a putative metabolite of primaquine, also underwent metabolism involving 3'-hydroxylation of the side chain. WR 6026, 8-(6-diethylaminoethylamino)-6-methoxy-4-methylquinoline, is an antileishmanial 8-aminoquinoline derivative. The in vitro metabolism of WR 6026 also results in the formation of side chain-oxygenated metabolites. The present results, together with previous observations on the metabolism of WR 238605 suggest that side-chain oxygenation is an important metabolic pathway of antiparasitic 8-aminoquinoline compds. in general.

IT 160924-73-2

RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)  
(sidechain hydroxylation in the metabolism of 8-aminoquinoline antiparasitic agents)

RN 160924-73-2 CAPLUS

CN 2-Pyrrolidinone, 1-(5,6-dihydroxy-8-quinolinyl)-3-hydroxy-5-methyl- (9CI)  
(CA INDEX NAME)



L19 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:307858 CAPLUS

DOCUMENT NUMBER: 122:95805

TITLE: Metabolism of a candidate 8-aminoquinoline  
antimalarial agent, WR 238605, by rat liver microsomes  
AUTHOR(S): Idowu, O. R.; Peggins, J. O.; Brewer, T. G.; Kelley,  
C.

CORPORATE SOURCE: Department Pharmacology, Walter Reed Army Institute  
Research, Washington, DC, 20307-5100, USA

SOURCE: Drug Metabolism and Disposition (1995),  
23(1), 1-17

CODEN: DMDSAI; ISSN: 0090-9556

PUBLISHER: Williams & Wilkins

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The in vitro metabolism of the 8-aminoquinoline, 8-(4-amino-1-methylbutylamino)-2,6-dimethoxy-4-methyl-5-(3-trifluoromethylphenoxy)quinoline (WR 238605), by rat liver microsomes was studied. After incubation of WR 238605 with rat liver microsomes, the metabolites were isolated either by direct solvent extraction or by extraction in

the presence of Et chloroformate. WR 238605 was extensively metabolized to aminophenolic compds., which underwent air oxidation during the isolation process to a mixture of quinones and quinone imines. Because of the instability of the metabolites toward air oxidation, most of them could only be isolated as the ethoxycarbonyl derivs. by in situ derivatization with Et chloroformate. The metabolism of WR 238605 involved the expected metabolic pathways, such as O-demethylation, N-dealkylation, N-oxidation, and oxidative deamination. In addition, C-hydroxylation involving the 8-aminoalkylamino side chain, which was previously unknown for 8-aminoquinoline analogs, was found to be an important metabolic pathway for WR 238605. Most of the metabolites retained the 5-(m-trifluoromethyl)phenoxy group of WR 238605. Direct and indirect supporting evidence for the structure of the metabolites of WR 238605 came from the concomitant study of the in vitro metabolism of six other compds. that are putative metabolites of WR 238605.

IT 160668-01-9

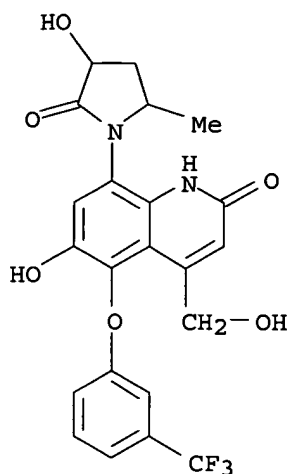
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)  
(metabolism of aminoquinoline antimalarial WR 238605 by rat liver microsomes)

RN 160668-01-9 CAPLUS

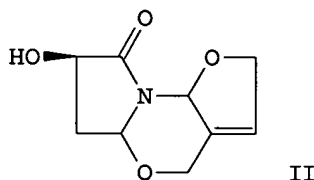
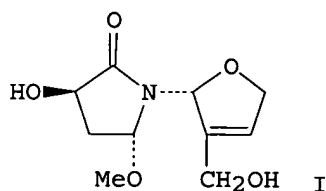
02/01/2005

10750247.trn

CN 2(1H)-Quinolinone, 6-hydroxy-4-(hydroxymethyl)-8-(3-hydroxy-5-methyl-2-oxo-1-pyrrolidiny)-5-[3-(trifluoromethyl)phenoxy]- (9CI) (CA INDEX NAME)



L19 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1994:431093 CAPLUS  
DOCUMENT NUMBER: 121:31093  
TITLE: 2,5-dihydrofuryl- $\gamma$ -lactam derivatives from  
Hemerocallis fulva L. var. kwanso Regel. II  
AUTHOR(S): Inoue, Tomohiroo; Konishi, Tenji; Kiyosawa, Shiu;  
Fujiwara, Yasuhiro  
CORPORATE SOURCE: Kyoto Pharm. Univ., Kyoto, 607, Japan  
SOURCE: Chemical & Pharmaceutical Bulletin (1994),  
42(1), 154-5  
CODEN: CPBTAL; ISSN: 0009-2363  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



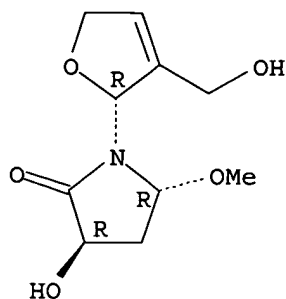
AB Two new 2,5-dihydrofuryl- $\gamma$ -lactam derivs., fulvanine D (I) and E (II), were extracted from Hemerocallis fulva L. var. kwanso Regel along with fulvanine A, B, and C. The structures of I and II were established as 1-(3-hydroxymethyl-2,5-dihydro-2-furyl)azacyclopenta-3-hydroxy-5-methoxy-2-one and 1,2,4,5,5a,6,7,8-8a,8b-decahydro-1,5-dioxa-8a-aza-asym-indacen-7-hydroxy-8-one.  
IT 155944-19-7  
RL: BIOL (Biological study)  
(from Hemerocallis fulva, structure of)  
RN 155944-19-7 CAPLUS

02/01/2005

10750247.trn

CN 2-Pyrrolidinone, 1-[2,5-dihydro-3-(hydroxymethyl)-2-furanyl]-3-hydroxy-5-methoxy-, [1(R\*),3 $\alpha$ ,5 $\beta$ ]-(-) - (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



L19 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:51776 CAPLUS

DOCUMENT NUMBER: 118:51776

TITLE: Disposition of the enantiomers of cromakalim in rat and cynomolgus monkey

AUTHOR(S): Tomlinson, P. W.; Ramji, J. V.; Filer, C. W.

CORPORATE SOURCE: SmithKline Beecham Pharm., The Frythe/Welwyn/Herts., AL6 9AR, UK

SOURCE: Xenobiotica (1992), 22(7), 799-814

CODEN: XENOBH; ISSN: 0049-8254

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Disposition of the 3R,4S(+) and 3S,4R(-) enantiomers of the racemic antihypertensive drug cromakalim has been studied in rats and cynomolgus monkeys using the <sup>14</sup>C-drug labeled in either the 3R,4S(+) or the 3S,4R(-) enantiomer. After oral administration to rat, blood concns. of the 3R,4S(+) enantiomer were up to 4-fold higher than those of the 3S,4R(-) enantiomer. Metabolism of the former was not as extensive as that of the latter and consequently plasma and urinary radiometabolite patterns were quant. different. In contrast to rat, there were much greater differences in the disposition of the two enantiomers following oral administration of cromakalim to the cynomolgus monkey. Plasma concns. of the 3R,4S(+) enantiomer were approx. 100 + those of the 3S,4R(-) enantiomer and the rate of urinary <sup>14</sup>C elimination for the 3R,4S(+) enantiomer was much faster than that for the 3S,4R(-) enantiomer. Plasma and urinary radiometabolite patterns were very different for the two isomers. Metabolite end products of the 3R,4S(+) enantiomer were predominantly phase I metabolites whereas the 3S,4R(-) enantiomer was almost entirely metabolized by glucuronidation. A study of the racemic drug alone would have led to a misunderstanding of the fate of the compound in these species.

IT 118628-73-2 145416-58-6 145416-59-7

RL: FORM (Formation, nonpreparative)

(formation of, as cromakalim enantiomeric metabolite, in cynomolgus monkey and rat)

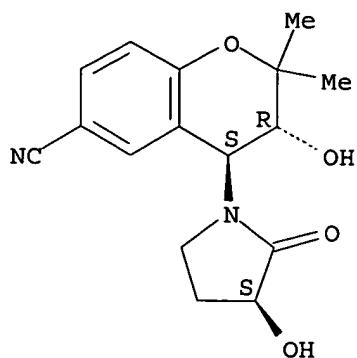
RN 118628-73-2 CAPLUS

CN 2H-1-Benzopyran-6-carbonitrile, 3,4-dihydro-3-hydroxy-4-(3-hydroxy-2-oxo-1-pyrrolidinyl)-2,2-dimethyl-, [3 $\alpha$ ,4 $\beta$ (S\*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

02/01/2005

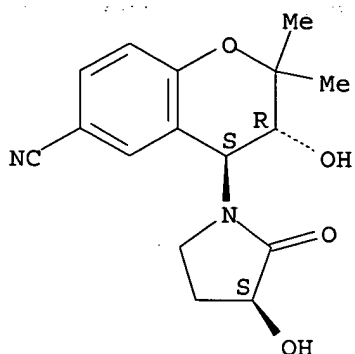
10750247.trn



RN 145416-58-6 CAPLUS

CN 2H-1-Benzopyran-6-carbonitrile, 3,4-dihydro-3-hydroxy-4-(3-hydroxy-2-oxo-1-pyrrolidinyl)-2,2-dimethyl-, [3R-[3α,4β(S\*)]]- (9CI) (CA INDEX NAME)

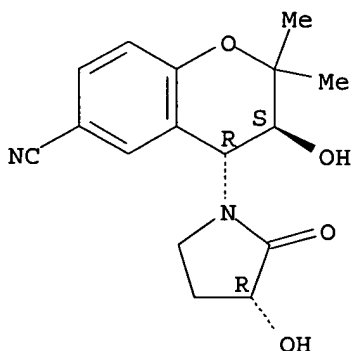
Absolute stereochemistry.



RN 145416-59-7 CAPLUS

CN 2H-1-Benzopyran-6-carbonitrile, 3,4-dihydro-3-hydroxy-4-(3-hydroxy-2-oxo-1-pyrrolidinyl)-2,2-dimethyl-, [3S-[3α,4β(S\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



02/01/2005

10750247.trn

L19 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:235638 CAPLUS

DOCUMENT NUMBER: 116:235638

TITLE: Preparation of 8-piperdiny-6H-pyrano[2,3-f]benzo-2,1,3-oxadiazoles as antihypertensives

INVENTOR(S): Seto, Kiyotomo; Matsumoto, Hiroo; Kamikawaji, Yoshimasa; Ohrai, Kazuhiko; Ohdoi, Keisuke; Sakoda, Ryoza; Masuda, Yukinori

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 31 pp.

CODEN: EPXXDW

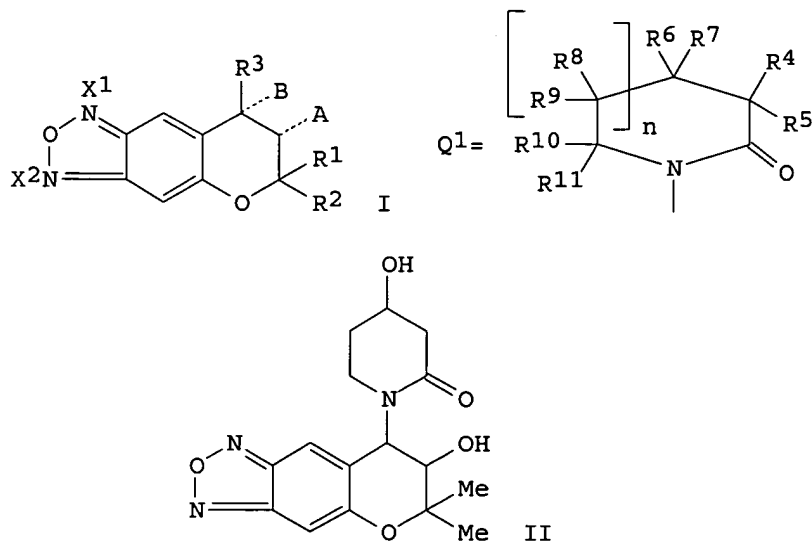
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 466131	A2	19920115	EP 1991-111490	19910710 <--
EP 466131	A3	19920304		
EP 466131	B1	19950927		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 04342591	A2	19921130	JP 1991-120279	19910524 <--
US 5272271	A	19931221	US 1991-726897	19910708 <--
CA 2046730	AA	19920111	CA 1991-2046730	19910710 <--
AT 128468	E	19951015	AT 1991-111490	19910710 <--
PRIORITY APPLN. INFO.:			JP 1990-182525	A 19900710
			JP 1991-120279	A 19910524
OTHER SOURCE(S):		MARPAT 116:235638		
GI				



AB Title compds. [I; X1, X2 = null, O; A = OH, acyloxy; B = H; AB = bond; R1, R2 = H, alkyl; R1R2 = (alkyl substituted) (CH2)<sub>m</sub>; m = 2-5; R3 = Q1, NR12R13, n = 0,1; R4-R11 = H, alkyl, ONO2, OSO3H, OH, acyloxy, alkoxy, trialkylsilyloxy, etc.; R12, R13 = H, alkyl, acyl; R12R13N = (substituted)

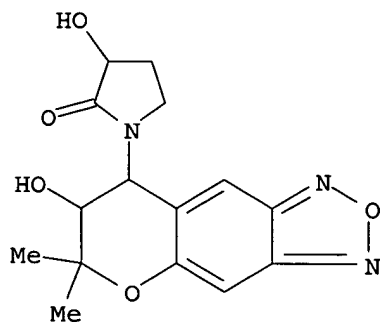
5-6 membered heterocycl[yl] were prepared (+)- $\beta$ -tert-Butyldimethylsilyloxy-8-valerolactone and (+)-7,8-dihydro-6,6-dimethyl-7-hydroxy-8-amino-6H-pyrano[2,3-f]benzo-2,1,3-oxadiazole were heated at 100° for 3h to give a mixture of diastereomeric amides. The diastereomers were separated followed by bromination with Ph<sub>3</sub>P/CBr<sub>4</sub>, cyclization with Et<sub>4</sub>NOH in DMF/Me<sub>2</sub>SO, and desilylation with Bu<sub>4</sub>NF in THF to give title compds. II. One isomer of II at 0.1 mg/kg orally gave 29% reduction in systolic blood pressure in spontaneously hypertensive rats. Several dosage formulations were prepared containing this isomer.

IT 140628-82-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of, as antihypertensive)

RN 140628-82-6 CAPLUS

CN 2-Pyrrolidinone, 1-(7,8-dihydro-7-hydroxy-6,6-dimethyl-6H-pyrano[2,3-f]-2,1,3-benzoxadiazol-8-yl)-3-hydroxy- (9CI) (CA INDEX NAME)



L19 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:234928 CAPLUS

DOCUMENT NUMBER: 114:234928

TITLE: Physicochemical properties and stability of  
tosulfloxacin tosylate

AUTHOR(S): Ohasi, Osamu; Kokei, Tetsuo; Shinmura, Tetsuzo;  
Takakura, Isamu

CORPORATE SOURCE: Toyama Kagaku Kogyo K. K., Japan

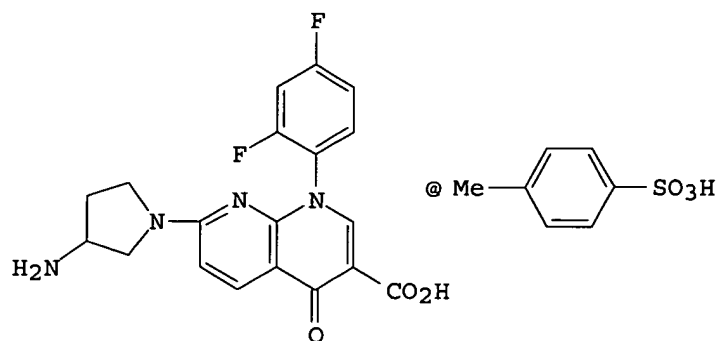
SOURCE: Kagaku Ryoho no Ryoiki (1990), 6(9), 1937-45

CODEN: KRRYEI; ISSN: 0913-2384

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

GI



AB The physicochem. properties (e.g. solubility, hygroscopicity, etc.) and stability in solns. and tablets of tosulfloxacin tosylate (I) were studied. I is stable for  $\geq 12$  mo in aluminum foils (PTP package) under ordinary storage condition; only slight color changes were noted, and the photodegrdn. product of I was identified.

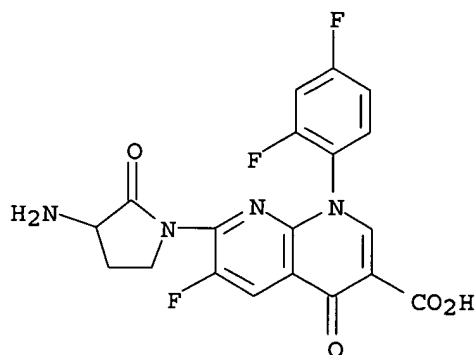
IT 133878-42-9

RL: FORM (Formation, nonpreparative)

(formation of, as photodegrdn. product of tosulfloxacin)

RN 133878-42-9 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 7-(3-amino-2-oxo-1-pyrrolidinyl)-1-(2,4-difluorophenyl)-6-fluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



L19 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:139787 CAPLUS

DOCUMENT NUMBER: 114:139787

TITLE: Novel 2,5-dihydrofuryl- $\gamma$ -lactam derivatives from *Hemerocallis fulva* L. var. kwanzo Regel

AUTHOR(S): Inoue, Tomohiro; Iwagoe, Kiyoshi; Konishi, Tenji; Kiyosawa, Shiu; Fujiwara, Yasuhiro

CORPORATE SOURCE: Kyoto Pharm. Univ., Kyoto, 607, Japan

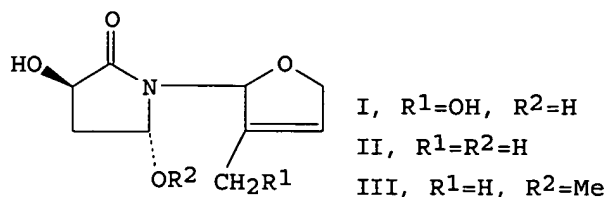
SOURCE: Chemical & Pharmaceutical Bulletin (1990), 38(11), 3187-9

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Three novel 2,5-dihydrofuryl- $\gamma$ -lactam derivs., fulvanine A (I), B (II), and C (III), have been extracted from *H. fulva* var. *kwanzo* along with oxypinnatanine. Their resp. structures have been established as 1-(3-hydroxymethyl-2,5-dihydrofuryl)-azacyclopenta-3,5-dihydroxy-2-one, 1-(3-methyl-2,5-dihydrofuryl)-azacyclopenta-3,5-dihydroxy-2-one, and 1-(3-methyl-2,5-dihydrofuryl)-azacyclopenta-3-hydroxy-5-methoxy-2-one.

IT 132922-40-8, Fulvanine A 132922-41-9, Fulvanine B

132922-42-0, Fulvanine C

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

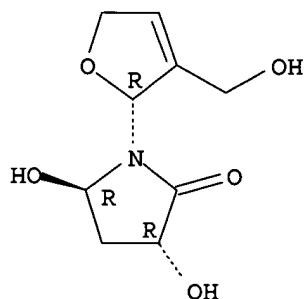
(of *Hemerocallis fulva*, isolation and structure determination of)

RN 132922-40-8 CAPLUS

CN 2-Pyrrolidinone, 1-[(2R)-2,5-dihydro-3-(hydroxymethyl)-2-furanyl]-3,5-dihydroxy-, (3R,5R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Currently available stereo shown.

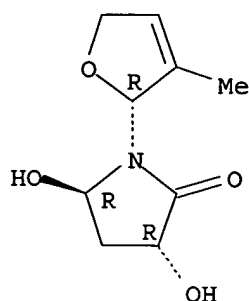


RN 132922-41-9 CAPLUS

CN 2-Pyrrolidinone, 1-[(2R)-2,5-dihydro-3-methyl-2-furanyl]-3,5-dihydroxy-, (3R,5R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Currently available stereo shown.

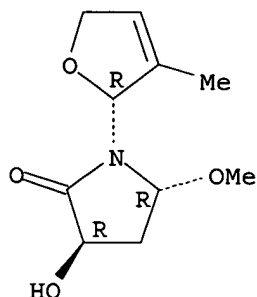


RN 132922-42-0 CAPLUS

CN 2-Pyrrolidinone, 1-[(2R)-2,5-dihydro-3-methyl-2-furanyl]-3-hydroxy-5-methoxy-, (3R,5R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Currently available stereo shown.



L19 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1989:173086 CAPLUS

DOCUMENT NUMBER: 110:173086

TITLE: Benzopyran compounds, processes for their preparation and their pharmaceutical use

INVENTOR(S): Cassidy, Frederick; Faruk, Erol Ali

PATENT ASSIGNEE(S): Beecham Group PLC, UK

SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

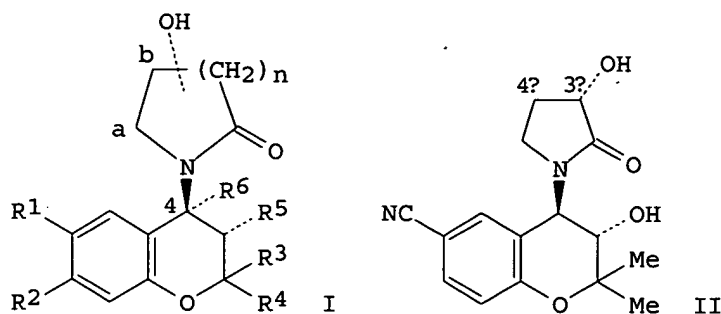
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 274821	A1	19880720	EP 1987-309235	19871019 <--
EP 274821	B1	19930303		
R: BE, CH, DE, JP 63165380	A2	19880708	JP 1987-265202	19871020 <--
US 4831050	A	19890516	US 1987-111770	19871021 <--
PRIORITY APPLN. INFO.: GB 1986-25185			GB 1986-25185	A 19861021
OTHER SOURCE(S): GI	MARPAT	110:173086		



AB Benzopyrans I [1 of R1, R2 = H and the other = alkyl-, alkoxycarbonyl, alkylcarbonyloxy, NO2, cyano, etc.; 1 of R1, R2 = NO2, cyano, alkylcarbonyl and the other = MeO or amino (un)substituted with 1 or 2 alkyl or by alkanoyl; 1 of R3, R4 = H or alkyl and the other = alkyl; R3R4 = polymethylene; either R5 = H, OH, alkoxy, or acyloxy and R6 = H or R5R6 = bond; n = 1,2; the OH group substituting the lactam group at other than position a; substituted lactam group is trans to R5 when R5 = OH, alkoxy, or acyloxy] or their salts, useful as antihypertensives, were prepared (±)-6-Cyano-3,4-dihydro-2,2-dimethyl-trans-3-bromo-4-hydroxy-2H-1-benzopyran in Me2SO was stirred with NaH 45 min to give a solution of the 3,4-epoxide which was cooled to .apprx.10° and treated with 3-(trimethylsilyloxy)-2-pyrrolidinone, NaH, and Me2SO to give a mixture containing .apprx.50% (±)-3'α-OH isomer (II) and .apprx.50% the corresponding 3'β-OH isomer. The (±)-4'α-OH isomer of II, at 10 mg/kg orally in spontaneously hypertensive rats caused 49±0, 46±5, 29±6, 40±5, and 5±3 mm lowering of systolic blood pressure after 1, 2, 4, 6, and 24 h, resp.

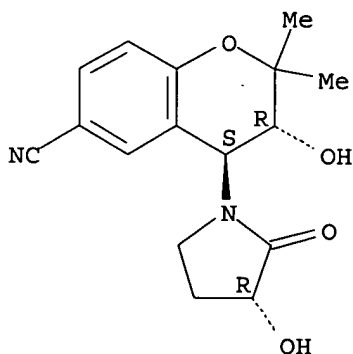
IT 118581-51-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as antihypertensive and potential agent for other cardiovascular disorders)

RN 118581-51-4 CAPLUS

CN 2H-1-Benzopyran-6-carbonitrile, 3,4-dihydro-3-hydroxy-4-(3-hydroxy-2-oxo-1-pyrrolidinyl)-2,2-dimethyl-, [3α,4β(R\*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 118628-73-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

02/01/2005

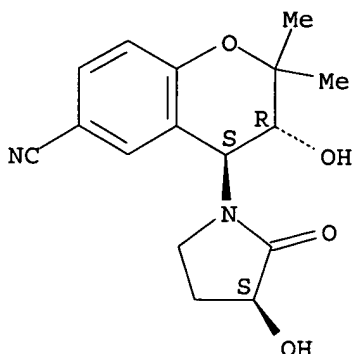
10750247.trn

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of, as cardiovascular agent)

RN 118628-73-2 CAPLUS

CN 2H-1-Benzopyran-6-carbonitrile, 3,4-dihydro-3-hydroxy-4-(3-hydroxy-2-oxo-1-pyrrolidinyl)-2,2-dimethyl-, [3 $\alpha$ ,4 $\beta$ (S\*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L19 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:461428 CAPLUS

DOCUMENT NUMBER: 109:61428

TITLE: A high-performance liquid chromatographic assay of the electrooxidation of purines. Uric acid and the nucleotide drug tubercidin-5'-monophosphate  
AUTHOR(S): Childers-Peterson, T.; Brajter-Toth, A.  
CORPORATE SOURCE: Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA  
SOURCE: Analytica Chimica Acta (1987), 202, 167-74  
CODEN: ACACAM; ISSN: 0003-2670

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:61428

AB A HPLC is described for establishing the completeness of electrooxidn. of a purine nucleotide drug, tubercidin-5'-monophosphate (TMP), and the sequence of product formation. TMP was completely oxidized after 2 h of electrolysis and the product distribution continued to change after this time. The same assay was also used to show the sequence of product formation in the electrooxidn. of uric acid. Both sepns. were isocratic, with a pH 4.6-5.1 0.02M KH<sub>2</sub>PO<sub>4</sub> mobile phase.

IT 113203-36-4

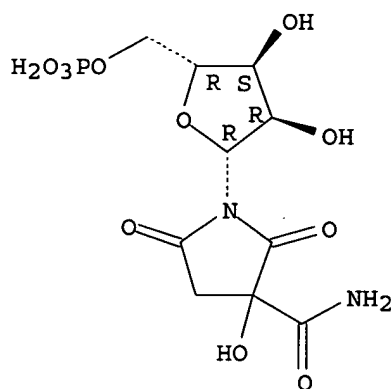
RL: BIOL (Biological study)

(tubercidin phosphate oxidation product, HPLC study of)

RN 113203-36-4 CAPLUS

CN 3-Pyrrolidinecarboxamide, 3-hydroxy-2,5-dioxo-1-(5-O-phosphono- $\beta$ -D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:120904 CAPLUS

DOCUMENT NUMBER: 108:120904

TITLE: Electrochemical and photochemical oxidation of the deazapurine nucleotide drug tubercidin-5'-monophosphate

AUTHOR(S): Childers-Peterson, Teresa E.; Brajter-Toth, A.

CORPORATE SOURCE: Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA

SOURCE: Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1988), 239(1-2), 161-73  
CODEN: JEIEBC; ISSN: 0022-0728

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Electrooxidn. of deazapurine nucleotide, tubercidin-5'-monophosphate (TMP), was investigated by cyclic voltammetry, coulometry and constant potential electrolysis. HPLC, mass spectrometry, FTIR and NMR spectroscopy were used to identify reaction intermediates and products. Photochem. oxidation of TMP was studied by HPLC and UV spectroscopy. Exptl. results show formation of the same products in the electrochem. and photochem. oxidation. The products that were identified indicate a possible radical oxidation pathway. The results demonstrate the role of adsorption in the electrochem. oxidation of TMP.

IT 113203-36-4P

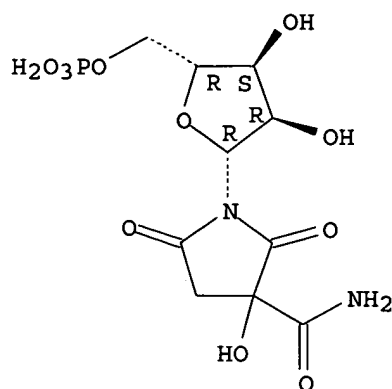
RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, during electrochem. and photochem. oxidation of tubercidin monophosphate in phosphate buffer solution)

RN 113203-36-4 CAPLUS

CN 3-Pyrrolidinecarboxamide, 3-hydroxy-2,5-dioxo-1-(5-O-phosphono-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1977:518030 CAPLUS  
 DOCUMENT NUMBER: 87:118030  
 TITLE: Stereoselectivity and reactivity in the 1,3-dipolar cycloaddition of chiral N-(alkoxyalkyl)nitrones  
 AUTHOR(S): Vasella, Andrea  
 CORPORATE SOURCE: Lab. Org. Chem., ETH, Zurich, Switz.  
 SOURCE: Helvetica Chimica Acta (1977), 60(4), 1273-95  
 CODEN: HCACAV; ISSN: 0018-019X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

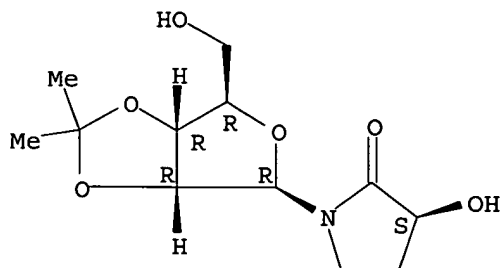
AB The ribofuranosylisoxazolidines I [R = H, R1 = R3 = Me, R2 = R4 (R5 = H); R = R3 = Me, R1 = H, R2 = R4 (R5 = H)] on treatment with N-chlorosuccinimide were cleaved to give isoxazolidines I [R = R2 = H, R1 = R3 = Me (II); R = R3 = Me, R1 = R2 = H (III)], resp. The trityl group did not influence the stereoselectivity in the cycloaddn. of D-ribose oximes IV (R6 = trityl, Me) with HCHO and CH2:CMCO2Me (V). Similarly, the cycloaddn. reactions of mannose oxime VI with RCOR1 (R = R1 = H, Me; R = H, R1 = Me) and V gave I (R-R2 = H, R3 = Me; R = R1 = R3 = Me, R2 = H), II, and III, possessing S-chirality at C-5, in 79-95% stereoselectivity. Both C-5 epimers of ribofuranosylisoxazolidines, R4R7 and R4R8 (R5 = H), were obtained by the reaction of IV (R6 = trityl) (VII) and paraformaldehyde with 1-octene and with cyclohexene, resp. The reaction of VII, HCHO, and CH2:CHCO2Me gave 57.9% (5S)-I [R = R1 = H, R2 = R4 (R5 = trityl), R3 = Me] and 32.4% of its 5R-isomer. The use of 2,3,4,6-tetra-O-methyl-D-glucose oxime permitted the synthesis of optically active isoxazolidines with regeneration of the starting hydroxy oxime.

IT 64018-70-8P 64018-71-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 64018-70-8 CAPLUS  
 CN 2-Pyrrolidinone, 3-hydroxy-1-[2,3-O-(1-methylethylidene)-β-D-ribofuranosyl]-, (S)- (9CI) (CA INDEX NAME)

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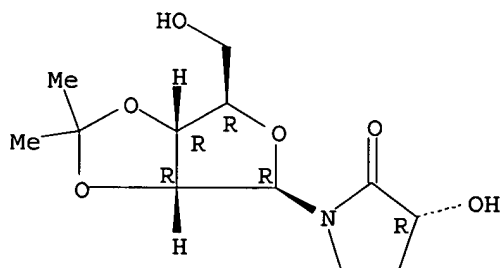
Absolute stereochemistry.



RN 64018-71-9 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[2,3-O-(1-methylethylidene)-β-D-ribofuranosyl]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:468562 CAPLUS

DOCUMENT NUMBER: 87:68562

TITLE: Synthesis and transformations of isoxazolidine nucleosides

AUTHOR(S): Vasella, Andrea

CORPORATE SOURCE: Lab. Org. Chem., ETH, Zurich, Switz.

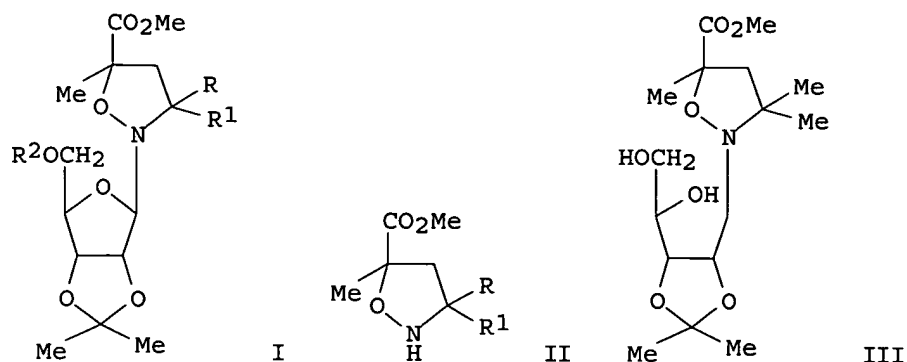
SOURCE: Helvetica Chimica Acta (1977), 60(2), 426-46

CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal

LANGUAGE: German

GI



AB Cyclocondensation of 2,3-O-isopropylidene-5-O-trityl-D-ribose oxime with  $\text{CH}_2:\text{CMeCO}_2\text{Me}$  and  $\text{RCOR}_1$  ( $\text{R} = \text{R}_1 = \text{H}$ ;  $\text{R} = \text{Me}$ ,  $\text{R}_1 = \text{H}$ ,  $\text{Me}$ ) gave the isoxazolidinylribosides I ( $\text{R} = \text{H}$ ,  $\text{Me}$ ;  $\text{R}_1 = \text{H}$ ,  $\text{Me}$ ;  $\text{R}_2 = \text{Ph}_3\text{C}$ ), which were treated with  $\text{FeCl}_3$  to give I ( $\text{R}_2 = \text{H}$ ). Treatment of I ( $\text{R} = \text{R}_2 = \text{H}$ ) and I ( $\text{R} = \text{R}_1 = \text{Me}$ ,  $\text{R}_2 = \text{H}$ ) with alcoholic  $\text{HClO}_4$  gave 84% II ( $\text{R} = \text{R}_1 = \text{H}$ ) and 67% II ( $\text{R} = \text{R}_1 = \text{Me}$ ), resp. Hydrogenolysis of I over Raney Ni followed by lactam formation gave the corresponding ribofuranosylpyrrolidinones, ribitolyl pyrrolidinones and the ribitolyl isoxazolidine III.

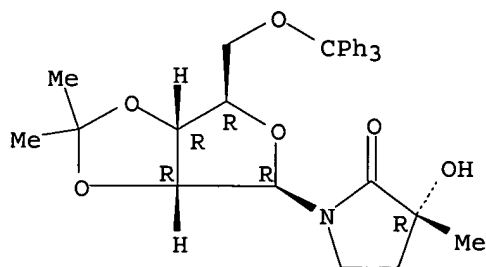
IT 63535-56-8P 63535-67-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)

RN 63535-56-8 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-3-methyl-1-[2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)- $\beta$ -D-ribofuranosyl]-, (R)- (9CI) (CA INDEX NAME)

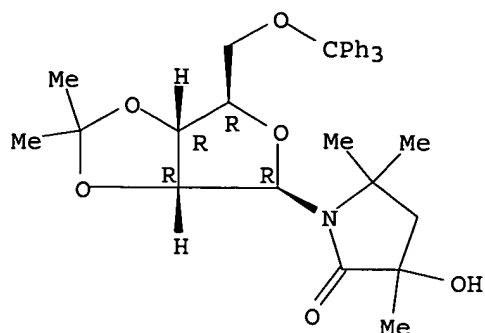
Absolute stereochemistry.



RN 63535-67-1 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-3,5,5-trimethyl-1-[2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)- $\beta$ -D-ribofuranosyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



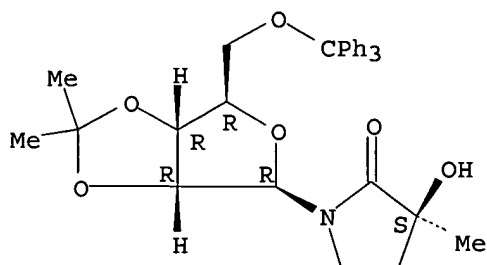
IT 63535-58-0P 63535-59-1P 63535-73-9P  
63549-78-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 63535-58-0 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-3-methyl-1-[2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-β-D-ribofuranosyl]-, (S)- (9CI) (CA INDEX NAME)

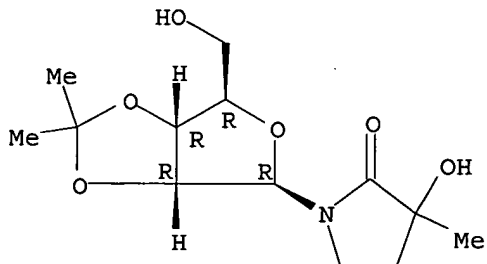
Absolute stereochemistry.



RN 63535-59-1 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-3-methyl-1-[2,3-O-(1-methylethylidene)-β-D-ribofuranosyl]- (9CI) (CA INDEX NAME)

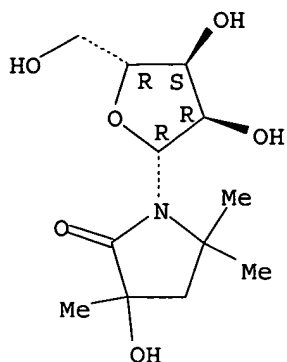
Absolute stereochemistry.



RN 63535-73-9 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-3,5,5-trimethyl-1-β-D-ribofuranosyl- (9CI)  
(CA INDEX NAME)

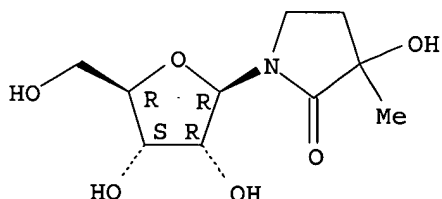
Absolute stereochemistry.



RN 63549-78-0 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-3-methyl-1-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:433426 CAPLUS

DOCUMENT NUMBER: 87:33426

TITLE: 3,4-Methylenedioxyphenyl-, isopropylidenedioxyphenyl-, and benzyl-substituted chiral 2-aminosuccinimides and 3-aminopyrrolidines. Stereoselective investigations of potential anti-Parkinsonian, antipsychotic, and anticonvulsant activities

AUTHOR(S): Witiak, Donald T.; Vishnuvajjala, Babu R.; Cook, Wayne L.; Minatelli, John A.; Gupta, Tribhuan K.; Gerald, Michael C.

CORPORATE SOURCE: Coll. Pharm., Ohio State Univ., Columbus, OH, USA

SOURCE: Journal of Medicinal Chemistry (1977), 20(6), 801-5

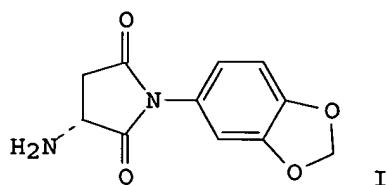
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 87:33426

GI



AB Seven enantiomeric pairs of title compds. were prepared by reaction of the appropriate aspartic acid derivative stereoisomer with 3,4-methylenedioxyaniline [14268-66-7], 3,4-isopropylidenedioxyaniline [6324-89-6], while the pyrrolidine enantiomers were prepared by reduction and alkylation of the corresponding benzylsuccinimide enantiomers. D-(R)-2-amino-N-(3,4-methylenedioxyphenyl)succinimide-HCl (I-HCl) [62396-38-7] partially attenuated amphetamine-induced stereotyped behavior in rats, while all the other compds. were inactive. D-(R)-2-amino-N-(3,4-isopropylidenedioxyphenyl)succinimide-HCl (II-HCl) [62396-40-1] antagonized oxotremorine-induced tremors in mice in a dose-dependent manner, while its enantiomorph was inactive. The median neurotoxic dose and time of peak activity, determined by the rotarod test, were similar for the various compds., but the D series was more active. Structure-activity relations are discussed.

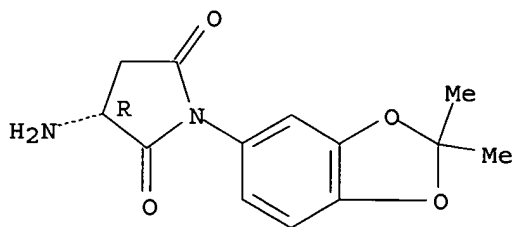
IT 62396-40-1P 62396-41-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(preparation and biol. activity of)

RN 62396-40-1 CAPLUS

CN 2,5-Pyrrolidinedione, 3-amino-1-(2,2-dimethyl-1,3-benzodioxol-5-yl)-, monohydrochloride, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

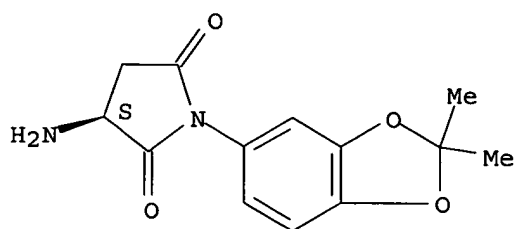


● HCl

RN 62396-41-2 CAPLUS

CN 2,5-Pyrrolidinedione, 3-amino-1-(2,2-dimethyl-1,3-benzodioxol-5-yl)-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

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L20 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:247333 CAPLUS

DOCUMENT NUMBER: 134:266475

TITLE: Preparation of quinuclidine compounds and drugs containing the same as the active ingredient of squalene synthase inhibitors

INVENTOR(S): Okada, Toshimi; Kurusu, Nobuyuki; Tanaka, Keigo; Miyazaki, Kazuki; Shinmyo, Daisuke; Sugumi, Hiroyuki; Ikuta, Hironori; Hiyoshi, Hironobu; Saeki, Takao; Yanagimachi, Mamoru; Ito, Masashi

PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan; et al.

SOURCE: PCT Int. Appl., 267 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

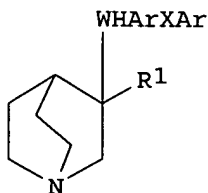
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

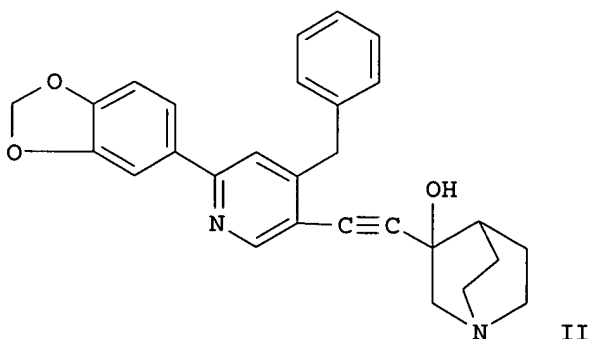
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001023383	A1	20010405	WO 2000-JP6665	20000927 <--
W: AU, BR, CA, CN, HU, IL, JP, KR, MX, NO, NZ, RU, US, ZA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2385995	AA	20010405	CA 2000-2385995	20000927 <--
AU 2000074464	A5	20010430	AU 2000-74464	20000927 <--
EP 1217001	A1	20020626	EP 2000-962889	20000927
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
BR 2000014331	A	20030610	BR 2000-14331	20000927
NZ 517788	A	20031128	NZ 2000-517788	20000927
ZA 2002002034	A	20030312	ZA 2002-2034	20020312
US 6599917	B1	20030729	US 2002-88554	20020319
NO 2002001528	A	20020528	NO 2002-1528	20020326
PRIORITY APPLN. INFO.:			JP 1999-273905	A 19990928
			JP 2000-179352	A 20000615
			WO 2000-JP6665	W 20000927

OTHER SOURCE(S): MARPAT 134:266475  
GI



I



II

AB Title compds. [I; wherein R1 is hydrogen or hydroxyl; HAr is an optionally substituted aromatic heterocycle; Ar is an optionally substituted aromatic ring;

W is a CH<sub>2</sub>CH<sub>2</sub> group which may be substituted, a CH:CH group which may be substituted, CC, NHCO, or the like; X is a single bond, optionally substituted C1-6 alkylene, Q ;wherein Q is oxygen, sulfur, CO, N(R<sub>2</sub>) ; wherein R<sub>2</sub> is C1-6 alkyl or C1-6 alkoxy, NHCO, or the like], salts thereof, or hydrates of both, are prepared and are useful as excellent squalene synthase inhibitors. Thus, the title compound II was prepared and tested.

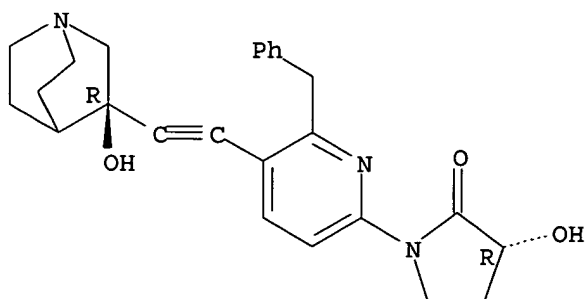
IT 332132-83-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of quinuclidine compds. and drugs containing the same as active ingredient of squalene synthase inhibitors)

RN 332132-83-9 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[5-[[[(3R)-3-hydroxy-1-azabicyclo[2.2.2]oct-3-yl]ethynyl]-6-(phenylmethyl)-2-pyridinyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 332135-05-4P 332135-10-1P

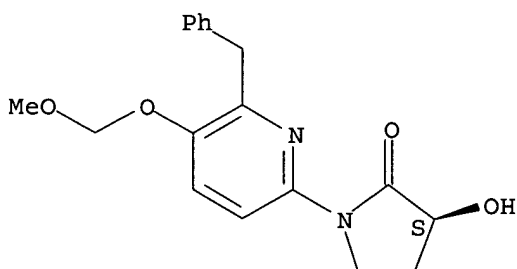
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of quinuclidine compds. and drugs containing the same as active ingredient of squalene synthase inhibitors)

RN 332135-05-4 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[5-(methoxymethoxy)-6-(phenylmethyl)-2-pyridinyl]-, (3S)- (9CI) (CA INDEX NAME)

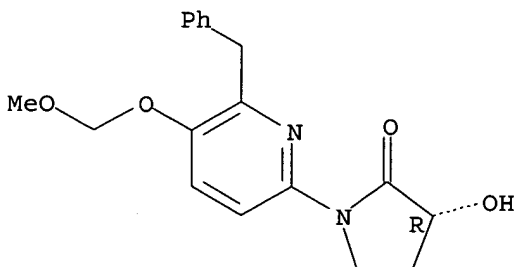
Absolute stereochemistry.



RN 332135-10-1 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[5-(methoxymethoxy)-6-(phenylmethyl)-2-pyridinyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 332132-82-8P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinuclidine compds. and drugs containing the same as active ingredient of squalene synthase inhibitors)

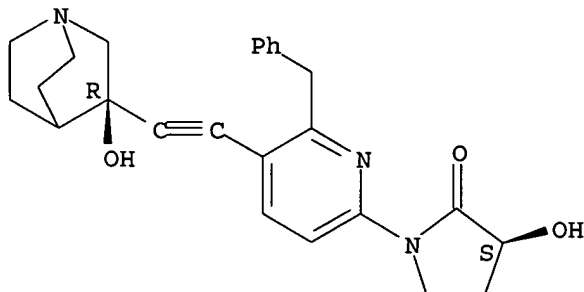
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RN 332132-82-8 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[5-[[[(3R)-3-hydroxy-1-azabicyclo[2.2.2]oct-3-yl]ethynyl]-6-(phenylmethyl)-2-pyridinyl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:260235 CAPLUS

DOCUMENT NUMBER: 132:293663

TITLE: Preparation of cyclopropylcarbonylaminopyrrolidinones, -thiazolidinones, or -oxazolidinones as herbicides.

INVENTOR(S): Parry, David Rees; Matthews, Ian Richard; Mitchell, Glynn; Williams, Alfred Glyn; Barnes, Nigel John; Cox, John Michael; Gillen, Kevin James; Ensminger, Michael Paul; Khodayari, Khosro; Nakayama, Hiroto

PATENT ASSIGNEE(S): Zeneca Limited, UK

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

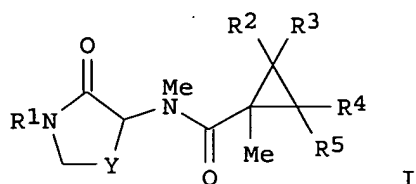
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000021928	A1	20000420	WO 1999-GB3143	19990921 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9961033	A1	20000501	AU 1999-61033	19990921 <--
BR 9914342	A	20010626	BR 1999-14342	19990921 <--
JP 2002527420	T2	20020827	JP 2000-575837	19990921
PRIORITY APPLN. INFO.:			GB 1998-22116	A 19981009
			WO 1999-GB3143	W 19990921

OTHER SOURCE(S): MARPAT 132:293663

GI

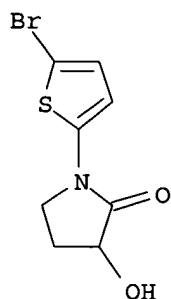


AB Title compds. [I; Y = O, S, CH<sub>2</sub>; R<sub>1</sub> = (substituted) aryl, heteroarom.; R<sub>2</sub>, R<sub>3</sub> = H, halogen; R<sub>4</sub>, R<sub>5</sub> = halo], were prepared **Thus**, 3-methylamino-1-(3-difluoromethoxy-4-methylphenyl)pyrrolidin-2-one (preparation given) in CH<sub>2</sub>Cl<sub>2</sub> was treated with 2,2-dichloro-1-methylcyclopropylcarbonyl chloride and then with Et<sub>3</sub>N to give diastereomeric 3-[N-(2,2-dichloro-1-methylcyclopropylcarbonyl)methylamino]-1-(3-difluoromethoxy-4-methylphenyl)pyrrolidin-2-one. Several I at 250 ppm preemergent gave 90-100% damage to *Amaranthus retroflexus*, *Echinochloa crus-galli*, etc.

IT **264194-57-2P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of cyclopropylcarbonylaminopyrrolidinones, -thiazolidinones, or -oxazolidinones as herbicides)

RN 264194-57-2 CAPLUS

CN 2-Pyrrolidinone, 1-(5-bromo-2-thienyl)-3-hydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:200115 CAPLUS

DOCUMENT NUMBER: 124:261022

TITLE: Preparation of substituted pyrrolidones, thiazolidones, or oxazolidones as herbicides

INVENTOR(S): Cox, John Michael; Clough, John Martin; Barnes, Nigel John; Pearson, David Philip John; Matthews, Ian Richard; Vohra, Shaheen Khatoon; Smith, Stephen Christopher; Mitchell, Glynn; Barber, Richard Anthony; Et, Al.

PATENT ASSIGNEE(S): Zeneca Ltd., UK

SOURCE: PCT Int. Appl., 221 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

02/01/2005

10750247.trn

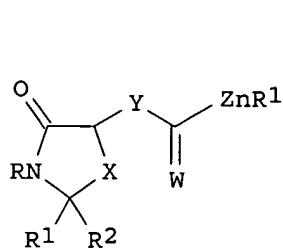
FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

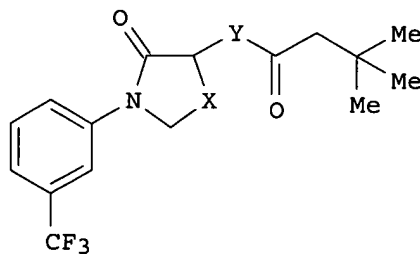
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WO 9533719	A1	19951214	WO 1995-GB1224	19950526 <--
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AU 9525720	A1	19960104	AU 1995-25720	19950526 <--
AU 696084	B2	19980903		
EP 763020	A1	19970319	EP 1995-920158	19950526 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
HU 75808	A2	19970528	HU 1996-3248	19950526 <--
CN 1153512	A	19970702	CN 1995-194250	19950526 <--
BR 9507838	A	19970916	BR 1995-7838	19950526 <--
JP 10500985	T2	19980127	JP 1995-500502	19950526 <--
ZA 9504443	A	19960205	ZA 1995-4443	19950531 <--
CN 1341594	A	20020327	CN 2001-125418	20010815
PRIORITY APPLN. INFO.:				
			GB 1994-10998	A 19940602
			GB 1994-11004	A 19940602
			GB 1995-1158	A 19950120
			WO 1995-GB1224	W 19950526

OTHER SOURCE(S): MARPAT 124:261022

GI



I



II

AB Title compds. [I; R = (un)substituted (hetero)aryl; R1 = H, hydrocarbyl, heterocyclyl, etc.; R2, R3 = H, alkyl; W = O or S; X = O, S, CR4R5; R4, R5 = H, alkyl; Y = O, S, NR6, CR4R5, etc.; R6 = H, OH, CHO, (di)(hydrocarbyl)amino, hydrocarbyl, etc.; Z = O, S, NR4, etc.; n = 0 or 1] were prepared Thus, 3-(F3C)C6H4NH2 was cyclocondensed with HSCH2CO2H and HCHO and the product converted in 2 steps to 5-hydroxy-3-(3-trifluoromethylphenyl)-4-thiazolidinone which was O-acylated with Me3CCH2COCl to give title compound II (X = S, Y = O). II (X = CH2, Y = NH) gave 90-100% control of 7 weeds, e.g., *Amaranthus retroflexus*, with 6-15% damage to soybean and corn and no damage to rice at 500g/ha preemergent.

IT 174889-59-9P 174889-68-0P 174889-87-3P

174889-88-4P 174889-89-5P 174889-90-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

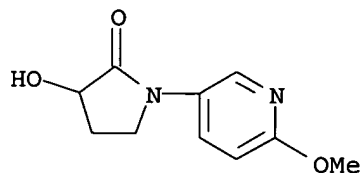
(preparation of substituted pyrrolidones, thiazolidones, or oxazolidones as herbicides)

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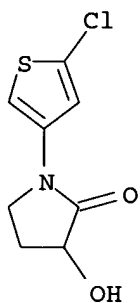
RN 174889-59-9 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-(6-methoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)



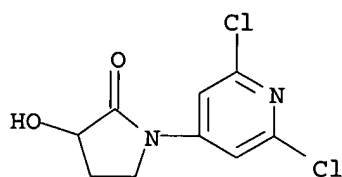
RN 174889-68-0 CAPLUS

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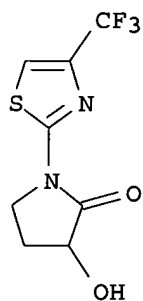
RN 174889-87-3 CAPLUS

CN 2-Pyrrolidinone, 1-(2,6-dichloro-4-pyridinyl)-3-hydroxy- (9CI) (CA INDEX NAME)



RN 174889-88-4 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[4-(trifluoromethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)

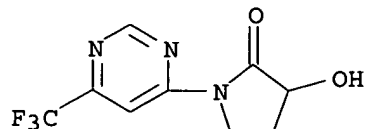


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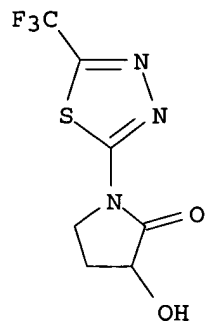
RN 174889-89-5 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[6-(trifluoromethyl)-4-pyrimidinyl]- (9CI)  
(CA INDEX NAME)



RN 174889-90-8 CAPLUS

CN 2-Pyrrolidinone, 3-hydroxy-1-[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]- (9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
115.61	929.78

SINCE FILE	TOTAL
ENTRY	SESSION
-16.06	-16.06

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